Henry's law constants measurements of the nonylphenol isomer 4(3′,5′-dimethyl-3′-heptyl)-phenol, tertiary octylphenol and γ-hexachlorocyclohexane between 278 and 298 K

Zhiyong Xie[a,b,*], Stéphane Le Calvé[c], Valérie Feigenbrugel[c], Thomas G. Preuß[d], Ralph Vinken[d], Ralf Ebinghaus[a], Wolfgang Ruck[b]

[a] *GKSS Research Centre, Institute for Coastal Research, Max-planck-str. 1, D-21502 Geesthacht, Germany*
[b] *Institute of Ecology and Environmental Chemistry at the University of Lueneburg, Scharnhorststr. 1, D-21335 Lueneburg, Germany*
[c] *Centre de Géochimie de la Surface, CNRS and Université Louis Pasteur, F-67084 Strasbourg cedex, France*
[d] *Institute for Biology V -Environmental Chemistry, Aachen University, D-52056 Aachen, Germany*

Abstract

Henry's Law Constants (HLC, $M\,atm^{-1}$) were determined for the diastereomeric mixture of the nonylphenol isomer 4(3′,5′-dimethyl-3′-heptyl)-phenol diastereomers (NP353(+) and NP353(−)), tertiary octylphenol (*t*-OP) and γ-hexachlorocyclohexane (γ-HCH) in artificial seawater over a temperature range 278–298 K using a dynamic equilibrium system. Trace organic substances present in the gas phase were trapped by tandem XAD-2 cartridges and extracted with a soxhlet extractor. The extracts were derivatived with N,O-bis(trimethylsilyl)-trifluoroacetamide (BSTFA), and then analyzed with GC-MS in the selective ion mode.

At 293 K and in artificial seawater, HLC ($M\,atm^{-1}$) were found to be equal to: NP353(+), HLC = (483 ± 169); NP353(−), HLC = (551 ± 193); *t*-OP, HLC = (400 ± 140); γ-HCH, HLC = (876 ± 307). The obtained data were used to derive the following Van't Hoff expressions: $\ln$ HLC (NP353(+)) = 8.73 (± 0.95) × (1000/T) −23.61 (± 3.30); $\ln$ HLC (NP353(−)) = 8.61 (± 0.91) × (1000/T)−23.08 (± 3.18); $\ln$ HLC (*t*-OP) = 9.03 (± 1.40) × (1000/T)−24.83 (± 4.86); $\ln$ HLC (γ-HCH) = 6.17 (± 1.08) × (1000/T)−14.28 (± 3.75). The derived enthalpies of solvation for NP353(+), NP353(−), *t*-OP and γ-HCH are −72.6 ± 7.9, −71.6 ± 7.6, −75.1 ± 11.5 and −51.3 ± 9.0 $kJ\,mol^{-1}$, respectively.

The HLC measurements of γ-HCH, which was used as reference substance, were in good agreement with literature values and its corresponding derived enthalpy of solvation agrees well to the previous values reported in the literature.

A reassessment of the air/water gas exchange based on experimentally derived HLC was made for the nonylphenol (NP) in the Lower Hudson River estuary (New York/New Jersey, USA) that was previously reported by Van Ry. A net atmospheric deposition was calculated for the gas exchange of NP in the Lower Bay ($Ff_w = 0.13$), and it nearly reaches the condition of equilibrium in the Upper Bay ($Ff_w = 0.46$).
© 2004 Elsevier Ltd. All rights reserved.

Keywords: Henry's law constant; Air/water exchange; Nonylphenol isomers; Tertiary octylphenol; γ-hexachlorocyclohexane

*Corresponding author. GKSS Research Centre, Institute for Coastal Research, Max-planck-str. 1, D-21502 Geesthacht, Germany.
E-mail address: zhiyong.xie@gkss.de (Z. Xie).

1. Introduction

For over 40 years, alkylphenol ethoxylates (APEOs), in particular nonylphenol ethoxylates (NPEOs, C_9H_{19}–C_6H_4–$(OC_2H_4)_n$–OH) have been applied in many